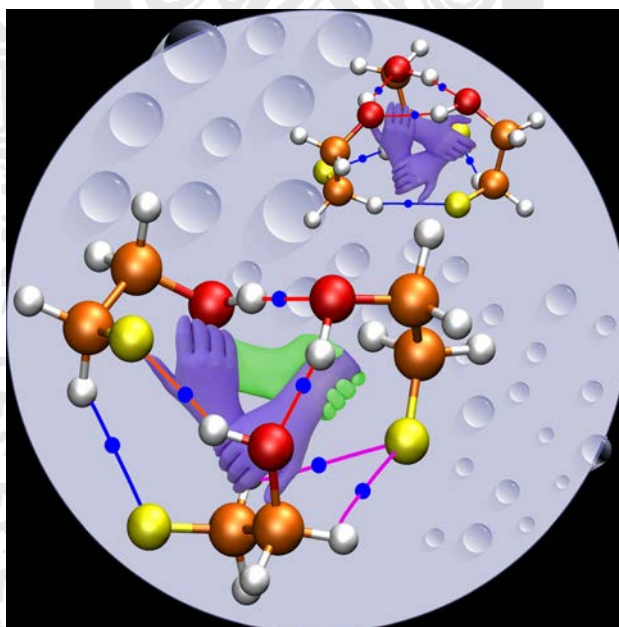


PHYSIKALISCHES KOLLOQUIUM UND IRTG-SEMINAR

(IRTG 2079: Cold Controlled Ensembles in Physics and Chemistry)



AM 2. MAI 2016 UM 17 UHR C.T.
IM GROßEN HÖRSAAL



SPECTRAL SIGNATURES OF CHIRALITY, CHIRALITY RECOGNITION, AND CHIRALITY TRANSFER

PROF. DR. YUNJIE XU

*DEPARTMENT OF CHEMISTRY, UNIVERSITY OF ALBERTA,
CANADA*

Chirality, or “handedness”, represents an intrinsic property of life. My research program focuses on applying and developing new spectroscopic tools to determine chirality and to establish chirality recognition models at the molecular level. In this presentation, I will first speak about high resolution spectroscopic studies of chirality recognition in several hydrogen-bonded clusters containing small transient chiral fluoroalcohols using both the cavity-based and chirped-pulse Fourier transform microwave techniques. Second, chiroptical spectroscopy, such as vibrational circular dichroism (VCD), can provide not only rich structural information of chiral molecules in solution, but also important insights into how they interact with each other and with solvent molecules. Our VCD results on transition metal complexes, amine borane complexes, and natural products in solution highlight the unique VCD sensitivity to solvent effects and hydrogen-bonding interactions. I will present our proposed “clusters-in-a-liquid” approach for simulating chiroptical spectra in water and in other solvents which can form H-bonds with a chiral solute. In particular, the link between VCD spectral signatures of small hydration clusters in the gas phase and in cold rare gas matrices and those obtained in aqueous solution will be discussed.